Modeling Multiscale-multiphase-multicomponent Subsurface Reactive Flows Using Advanced Computing

Peter Lichtner, Chuan Lu, EES-6; David Moulton, Bobby Philip, T-7

It is becoming increasingly clear that the ability to model multiscale subsurface processes is essential for obtaining an accurate predictive capability of contaminant transport [1]. Predictive modeling of reactive flows is a daunting task because of the wide range of spatial scales involved—from the pore to the field scale—ranging over more than six orders of magnitude, and the wide range of time scales involved—from seconds or less to millions of years. However, even with ultrascale (petascale and beyond) computing facilities, large 3D field scale continuum models employing billions of nodes on uniform grids can only resolve features on the order of tens of meters and cannot capture phenomena at much smaller scales on the order of centimeters to millimeters or less. Heterogeneity, multiphase interfacial effects, and multicomponent geochemical reactions add further complexity to the system requiring advances in modeling capabilities.

To meet these challenges, algorithms scaleable to large numbers of processors (>10,000) are needed to provide efficient simulation on ultrascale computing platforms. Adaptive mesh refinement (AMR) will be essential to limit the number of nodes needed to adequately represent the spatial variability of the system. And subgrid scale models will be essential to capture multicontinuum effects involving fracture-rock matrix interaction, preferential flow paths, and other multiscale phenomena. Implicit in applications of AMR to heterogenous media is the need for upscaling (e.g., permeability tensor) to model reactive flows at different resolutions.

These enhanced modeling capabilities will be used to improve our understanding of radionuclide migration at the DOE Hanford facility, where sub-millimeter-scale mass transfer effects have thwarted attempts at remediation efforts, and modeling sequestration of CO_2 in deep geologic formations, where resolving density-driven fingering patterns is necessary to accurately describe the rate of dissipation of the CO_2 plume. The focus of this highlight is on the challenges facing modeling CO_2 sequestration in geologic formations.

CO_2 Sequestration in Saline Aquifers. CO_2 sequestration (capture, separation, and long-term storage) in various geologic media including depleted oil reservoirs, saline aquifers, and oceanic sediments is being considered as a possible solution to reduce greenhouse gas emissions. Sequestration in subsurface geologic formations containing saline aquifers could provide permanent storage and thereby help mitigate global climate change. Saline aquifers have an estimated world-wide storage capacity for CO_2 of 100-10,000 Gt CO_2 [2].

Injection of supercritical CO_2 into deep underground reservoirs introduces unique computational challenges. At appropriate *p-T* conditions, supercritical CO_2 is buoyant because of its lower density compared with the brine, and rises, eventually becoming trapped by a caprock and spreading laterally as it gradually dissolves into the surrounding brine. As the CO_2 dissolves into the brine, however, the brine becomes heavier and begins to sink, resulting in density-driven convective instabilities leading in the formation of CO_2-concentrated brine fingers protruding downward. Convective mixing can result in much more rapid dissipation of the supercritical CO_2 plume compared with diffusive processes alone. Also important is the areal extent of the plume, which can increase the accidental release of CO_2 to the surface through abandoned bore holes and faults. Competition between the rate of spreading of the plume and the rate at which it dissolves into the brine controls the extent of spreading, and this competition is a complex multiscale process that is difficult to model.

Massively Parallel Multiphase Code PFLOTRAN. To investigate the role of convective mixing numerically, the massively parallel computer code PFLOTRAN is used to model multiphase-multicomponent processes involved in sequestration [3]. PFLOTRAN provides for phases of CO_2 and brine under nonisothermal conditions. Phase transformations are described using a variable switching approach as the thermodynamic state of a grid block changes from brine, to two phases: CO_2–brine, to pure CO_2.

The role of fingering on dissipation of a CO_2 plume is investigated numerically by injecting supercritical CO_2 into a highly permeable sandstone formation. As demonstrated in Fig. 1, the evolving profile of dissolved CO_2 is highly dependent on resolution of the fingers produced following the injection process. Fingering will also be important in determining chemical interactions between between reservoir minerals and the CO_2-enhanced brine.

For more information contact Peter Lichtner at lichtner@lanl.gov.

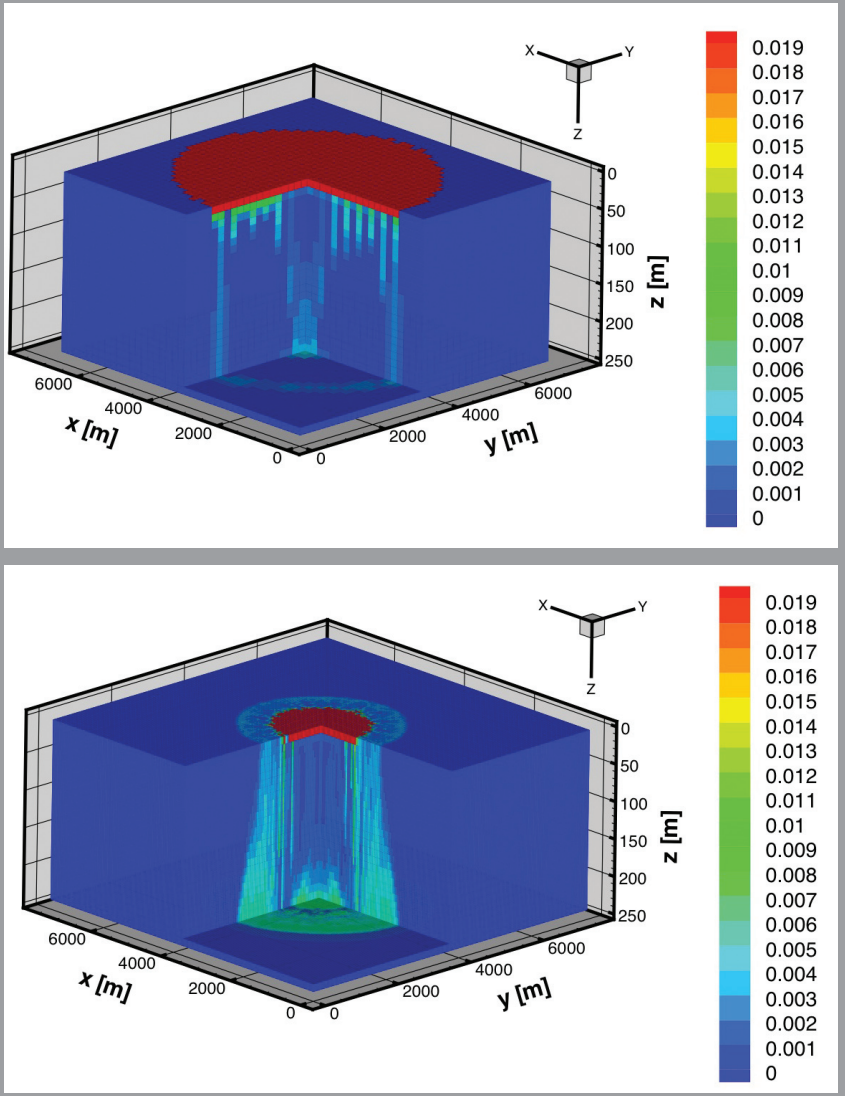

Fig. 1. Simulations carried out using PFLOTRAN showing dissolved CO_2 at an elapsed time of 300 years illustrating the dependence of fingering on coarse (top) and fine (lower) grid resolutions. The coarse grid consists of 40 x 40 x 25 nodes with spacing Dx = Dy -175 m and Dz = 10 m. The fine grid is refined in the x and y directions by a factor of four. An isotropic permeability of 2 x 10^{-12} m^2 is used with a porosity of 15% typical of sandstone. The computational domain is 250 m thick and 7 x 7 km in lateral extent. CO_2 is injected at a rate of 1 MT/y for 20 years at a depth of 50 m below the top of the domain, corresponding to roughly 75% of the CO_2 produced by a 1000 MW gas-fired power plant in 20 years. No-flow boundary conditions are imposed at the top and bottom and front and back of the domain, and with constant pressure at the left and right sides.

[1] Basic research needs for geosciences: facilitating 21 st century energy systems. Workshop sponsored by the U.S. Department of Energy, Office of Basic Energy Sciences, Feb 2007. (http://www.sc.doe.gov/bes/reports/list.html).
[2] Ibid.
[3] C. Lu, and P. Lichtner, *Journal of Physics Conference Series*, **78**, 012042 doi:10.1088/1742-6596/78/1/012042 (2007).

Funding Acknowledgments
- Department of Energy, Office of Science, Scientific Discovery through Advanced Computing Program
- Department of Energy, Office of Science, Innovative and Novel Computational Impact on Theory and Experiment Program